

**Escape of Martian Water:
Modeling the Atmosphere from the Surface to the Exobase**

A Proposal from Boston University to NASA – Mars Fundamental Research

To be submitted to NASA - 8 April 2004

PI: John T. Clarke

Collaborators: Michael Mendillo, Paul Withers, Jody Wilson, Jeffrey Forbes

Abstract:

Water has had a major impact on the martian surface and climate, and understanding the history of water is a major scientific goal of NASA's Mars Exploration Program. While there is ample and increasing evidence that the ancient Mars had copious amounts of water on its surface, there is no general understanding of how much of that water remains sequestered in the martian crust today, and how much may have escaped to space over time. While several groups have modeled the escape processes from the upper martian atmosphere, water molecules must be dissociated in the lower atmosphere, and the diffusion of their byproducts from the surface to the exobase (where they can escape into space) is subject to many factors. We here propose an extension of previous observational and modeling programs related to the martian atmosphere to develop a model which will include all of the key elements of the escape of martian water from the surface into space. We will adapt an existing finite-element simulation code, presently used to model the martian ionosphere, to extend down to the surface. This will treat the dissociation of water, including the varying rates of photo-induced and condensation-induced fractionation of deuterated species, their diffusion into the upper atmosphere, their chemistry (lower atmosphere) and photochemistry (upper atmosphere), and their energy-dependent escape from the exobase. Armed with a physics-based model of the entire atmosphere, it will then be possible to simulate conditions in the history of Mars, and determine the rates and main factors which have controlled the escape of martian water.

Table of Contents:

Summary of Personnel and Work Efforts:

Scientific/Technical/Management Section:

Introduction:

Atmospheric escape occurs on all three of the atmosphere-bearing terrestrial planets (Venus, Earth, Mars), and is the one of the major pathways for altering the climate of a planet (e.g. Chamberlain and Hunten 1987). Many of the physical processes leading to atmospheric escape are not well understood, which impedes our understanding of the past climates of Venus and Mars (Hunten 1993). Observations of an elevated deuterium to hydrogen ratio in the martian atmosphere, geological evidence for immense catastrophic flood channels, and integrated surface networks of dendritic drainage and valley systems strongly suggest that Mars once had a much wetter climate (Baker 2001; Jakosky and Phillips 2001). This has implications for the accretion of its volatile inventory during the formation of the solar system, its subsequent geological and thermal evolution, and its potential habitability (Jakosky and Phillips 2001; Owen 1992). For these and other reasons, understanding the history of water on Mars is a major goal of NASA's Space Science Enterprise which has been repeatedly endorsed by the reports of advisory boards such as COMPLEX, the Office of Space Science's Space Science Advisory Committee, and the National Academy of Science's Solar System Exploration Decadal Survey (COMPLEX 2001; Belton et al. 2002; SScAC 2004). "Follow the water" is the guiding theme of NASA's Mars Exploration Program.

Mars's initial volatile inventory would have formed a thick, hot atmosphere enveloping the molten planet as it grew. Much of this initial inventory would have been lost due to the low gravity, extended spatial scale of the hot atmosphere, and repeated impact erosion. Volatiles delivered late in the accretion process by the precursors of comets or asteroids would have been less susceptible to loss to space owing to the calmer environment that followed the fiery main phase of accretion. Only at this stage in martian history does the accumulation of volatiles become much less important than the loss of volatiles. One can regard this "late veneer" of volatiles as the initial state of today's atmosphere, although loss to space and the planetary interior have made today's atmosphere a wispy remnant of that initial state. Escape of water from Mars today does not take place by the loss of individual water molecules. Instead, these molecules are photo-dissociated in the lower atmosphere, and the lighter fragments (mainly H₂, HD, and O) are transported upwards. The present escape rates of these fragments were at first thought to be balanced such that the net effect is the loss of water molecules (McElroy 1972) maintaining the planet's oxidation state. However, Viking measurements of topside ion densities suggested that the oxygen escape flux is nearly an order of magnitude lower than that for hydrogen (Fox 1993). The resolution of this situation is not clear at this time.

Since its formation, volatiles such as H, C, N, O, and the heavier noble gases have been lost from the top of the martian atmosphere. Jeans escape, hydrodynamic blowoff, impact erosion, stripping by the solar wind (pick-up ion sputtering), and dissociative recombination production of hot fragment atoms can all remove atmospheric species from the top of the atmosphere. The efficiency of impact erosion is determined by the rate and size of impactors, an important process in the early history of Mars but less important in the last 3 Gyrs. This process also removes atmospheric species in bulk, without any differentiation with mass or isotope, but it is a weak contributor to the overall escape today. The efficiency of Jean's and some non-thermal

escape depends on the incident solar UV flux and atmospheric chemistry and diffusion. These processes will be modeled in detail in the proposed work. The efficiency of solar wind stripping of species depends on the solar wind pressure and field strength (Johnson and Luhmann 1998), the atmospheric composition with altitude, and the strength of any martian intrinsic field or remnant fields. This interaction is being studied in detail by a separate NASA-funded program to apply an Earth-based MHD code to the martian interaction (M. Mendillo and J. Schoendorf). The processes of Jean's and non-thermal escape and solar wind sputtering dominate present-day escape. These same processes are assumed to have operated on all solar system atmospheres, yet we do not have accurate quantitative models for how any solar system atmosphere has lost volatiles to space over geological time. Since Mars has weak gravity and a weak magnetic field, it should be more strongly affected at present by escape processes than Venus or the Earth.

Observations of the D/H ratio on Mars and Venus indicate an enhancement of factors of roughly 5 (Mars) and 150 (Venus) compared with the Earth (Owen 1992; Donahue et al. 1997). Assuming that hydrogen results principally from the dissociation of water, and that H escapes faster than D due to the mass difference, the present D/H ratio can be related to the total amount of water lost into space *if* one has an accurate understanding of the escape processes and diffusion of species from the lower atmosphere to the exobase. However, the D/H ratios in the upper atmospheres of Mars and Venus are much lower than the ratios in their bulk atmospheres, indicative of fractionation effects in the diffusion of species to the upper atmosphere (Bertaux and Clarke 1990; Bertaux et al. 1992; Krasnopolsky et al. 1998). To quote a Science magazine news and views article (Yung and Kass 1998) titled "Deuteronomy?: A Puzzle of Deuterium and Oxygen on Mars", it was stated: "...why we need to learn about the history of the martian climate. The reason is that Mars can be viewed as a laboratory where drastic climate change experiments were carried out, and because it does not have plate tectonics, the records of the experiments (written in the language of isotopic fractionations) are preserved. Similar evidence on Earth has been continually destroyed by tectonics and reequilibration. Metaphorically, the tablets of Moses have been wiped clean by planetary processes. Deuteronomy (The Second Giving of the Law) may be found in the Temple of another planet."

Previous models (Krasnopolsky 2002; Fox 1993) have generally restricted their region of interest to altitudes above the homopause, which is the altitude above which molecular diffusion dominates over large-scale mixing and eddy diffusion to cause separation of atmospheric species. This simplification allowed these models to focus on the regions from which escape occurred, but did not consider the resupply of escaped species to the exosphere. Fox (2003) and other workers have shown that predicted escape rates are very sensitive to such parameters as assumed H₂ concentration at the lower boundary. We propose here to develop an integrated picture in which the entire atmosphere is considered. Some previous models (Krasnopolsky et al. 1998; Bertaux and Montmessin 2003) have considered this bottleneck in the lower atmosphere, but have focused on limited numbers of species or limited numbers of escape mechanisms. This model will be the first to span from the surface to space while including a full range of species and escape mechanisms.

The result of the proposed modeling will be the capability to predict rates of escape from the martian atmosphere for different assumed conditions, for comparison with measurements from existing and future missions. Mars Express, supported by NASA as a "Mission of

"Opportunity", is making a number of observations relevant to escape. The existence and distribution of many minor species in the lower atmosphere will be determined by SPICAM (H₂O and O₃) and PFS (simple organic molecules such as CH₄). The basic structure of the upper atmosphere will be determined by SPICAM profiles of CO₂ density below 160 km. The interaction of escaping species and the solar wind will be studied by ASPERA's charged particle and energetic neutral atom detectors. Atmospheric densities in the exobase region as determined by MRO aerobraking will also affect our modeling of escape. The "New Frontiers in Solar System Exploration" Decadal Survey recommended a "Mars Aeronomy Orbiter" mission, which is present in NASA's pathways for Mars Exploration after 2009. The 2009 Mars Telecom Orbiter, if it carries a scientific payload, will be well-suited to observations of atmospheric escape over a substantial fraction of the solar cycle. Predictions of escape from our work can be used to support the designs of such missions and definition of their strawman payloads and instrument requirements.

The proposed work is responsive to and relevant to the overarching scientific research directions of the Mars Exploration Program, as summarized in the July 2001 Mars Exploration Payload Analysis Group (MEPAG) report in JPL Document 01-7:

- I.A.1 Map the three-dimensional distribution of water
- I.C.2 Determine the changes in atmospheric inventories of carbon over time
- II.A.1 Determine the processes controlling the present distributions of water, carbon dioxide, and dust
- II.A.4 Determine the rates of escape of key species from the martian atmosphere, and their correlation with solar activity and lower atmospheric phenomena

It is also relevant to the numbered priorities of the recent Space Studies Board report of the Committee for Planetary Exploration (COMPLEX) "Assessment of Mars Science and Mission Priorities" (2001) (2) Hot atom abundances and escape fluxes and (3) Ion escape from Mars. In addition, the proposed work is directly responsive to several NASA Goals and Research Focus Areas (RFAs) as stated in the latest version of its Strategic Plan: Goal II, SSE Objective 4, RFAs (a) and (b); Goal II, SEC Objective I, RFA (c). It also relates indirectly to Goal II, SSE Objective 1, RFAs (b) and (c); Goal II, SSE Objective 2, RFA (a).

Proposed Research Program:

While gases escape from the "top" of the martian atmosphere (the exobase, or the altitude where the collisional mean free path equals the scale height), a comprehensive modeling of that process must start far below the exosphere. Ideally, a "whole atmosphere" model, such as the one being developed for the terrestrial atmosphere at NCAR in Boulder, should be developed for Mars. For Earth, with its host of weather patterns, severe storms and ocean-atmosphere interfaces to consider in upward coupling scenarios, there is an obvious need for a rigorous surface-to-exosphere model. Yet for Mars, a planet without a troposphere, there are approaches to be used that are far less intense from a computational (and physical) basis. We propose here the development one such approach to study the upward propagation of trace species through the full martian atmosphere. We will adapt an existing finite-element simulation code, presently used to model the martian ionosphere, to extend down to the surface. This will treat the

dissociation of water, including the varying rates of photo-induced and condensation-induced fractionation of deuterated species, their diffusion into the upper atmosphere, their chemistry (lower atmosphere) and photochemistry (upper atmosphere), and their energy-dependent escape from the exobase. Armed with a physics-based model of the entire atmosphere, it will then be possible to simulate conditions in the history of Mars, and determine the rates and main factors which have controlled the escape of martian water.

As shown in Figure 1, the vertical structure of the martian atmosphere is simpler than that of Earth's. It effectively consists of a surface-bounded stratosphere, where temperatures decrease as altitude increases, transitioning into a thermosphere, where temperatures increase as altitude increases, near 100 km. This is analogous to the Earth's atmosphere above the complications of the troposphere and the ozone layer. The homopause (the altitude where eddy diffusion equals molecular diffusion) occurs at 120 - 140 km altitude and the exobase (the altitude where the mean free path equals the scale height) occurs at 200 - 250 km altitude. In the ionosphere, photochemical processes dominate below 170 - 200 km and transport processes dominate above that altitude. Photochemistry and diffusion of neutrals in the lower atmosphere will be modeled in the same formalism as in our existing model for photochemistry and diffusion in the ionosphere. Only the reactions and diffusion coefficients will be different. We will adopt the diffusion coefficients of Nair et al. (1994) plotted in Fig. 1 below.

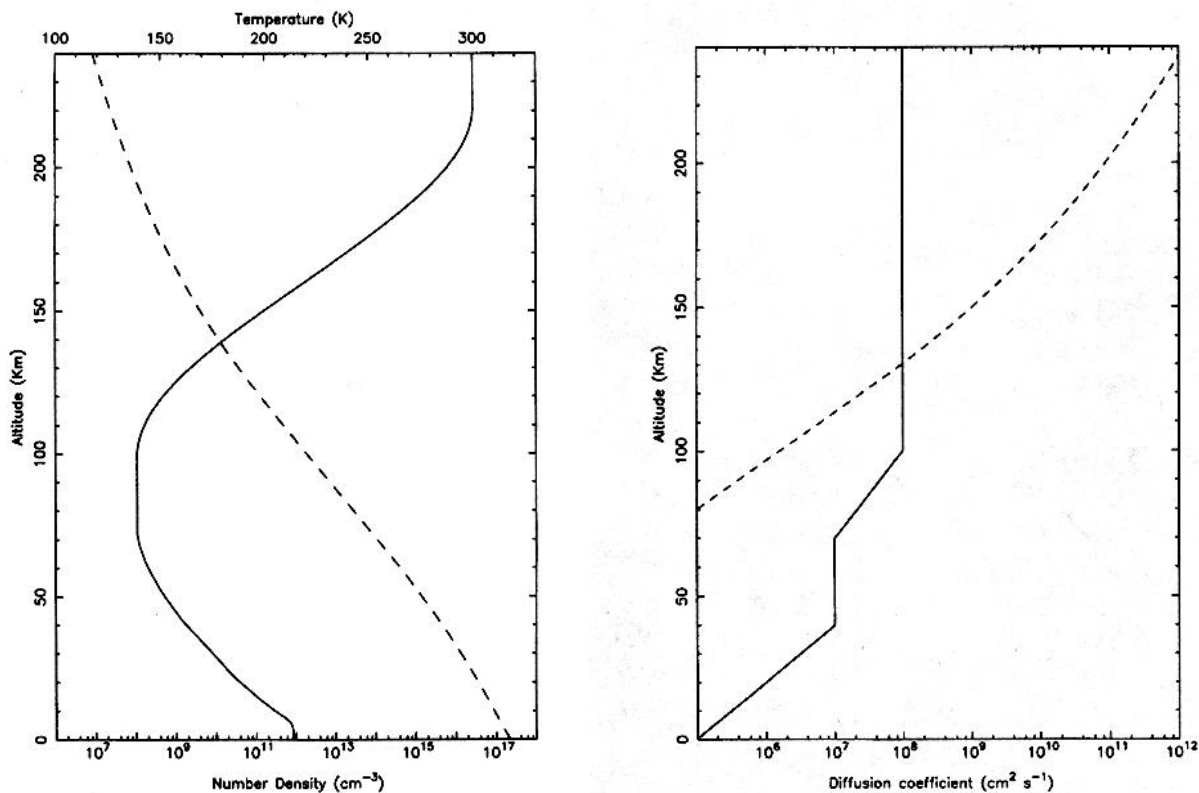


Figure 1: Model for the martian atmospheric density (dashed) and temperature (solid) and eddy (solid) and molecular (dashed) diffusion coefficients from Nair et al. (1994). These model values will be used in the proposed work for the lower atmosphere $z < 80$ km.

As a starting point for the structure of the lower atmosphere, we will require the total number density in the model to match the profile shown in Figure 1. We will specify mixing ratios of CO_2 , N_2 , and H_2O at the surface, then allow chemistry and transport to generate vertical profiles of each of these species and their reaction products, which include CO , O_2 , O_3 , OH , H , H_2 , and so on. Lower boundary conditions will be zero flux for all species. Upper boundary conditions at the exobase will be derived from the Monte Carlo escape model described below.

The basic inputs into our model will be an assumed background atmospheric structure, an incident solar spectrum, and a quantity of water (nominally a 10 prec. μm column). We will initially assume an atmosphere clear of dust, and may later add some dust opacity as a free parameter. These parameters can be varied according to the season and solar activity under consideration. Starting from the bottom of the atmosphere for ease of discussion, water may undergo a variety of chemical reactions (e.g. Barth et al. 1992, and Figure 2), may condense into discrete clouds or extended hazes, and may be transported vertically by turbulent mixing or diffusion. Solar photons will be absorbed, initiating reactions and releasing energy, by the background atmosphere. Some of these processes, including cloud formation and UV absorption, will affect deuterated species differently than non-deuterated species, and we will track the two main isotopes of hydrogen separately at all stages of the model (Krasnopolsky 2002; Bertaux and Montmesson, 2001). At higher altitudes, short-wavelength solar radiation will form photochemical ions leading to an ionosphere. Diffusive separation will commence at the homopause when coefficients of molecular diffusion for species exceed the bulk coefficient of eddy diffusion that is used to model large-scale mixing and turbulent processes. Above the exobase, molecular collisions cease to be important, continuum fluid dynamics no longer applies, and the trajectories of individual atoms and molecules have to be modeled ballistically.

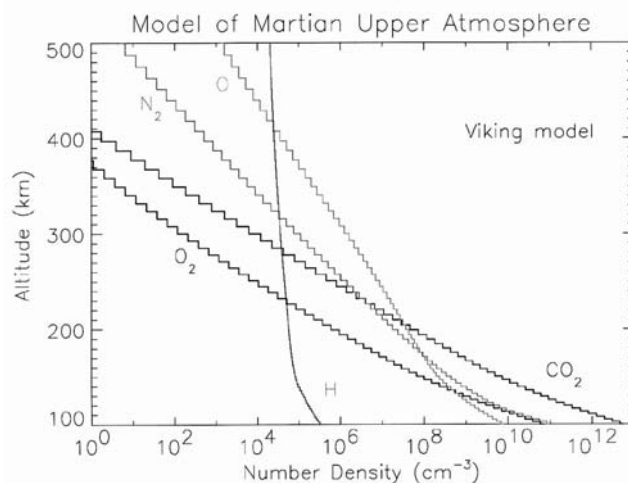
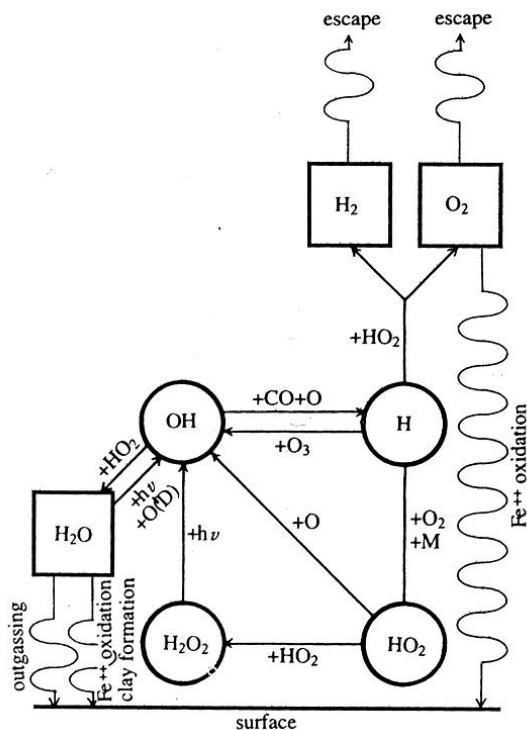


Figure 2: Cartoon of water chemistry (left) from Lewis (1997), and (right) Viking model for the martian upper atmosphere (Nier and McElroy 1977).

While our team has considerable experience in atmospheric structure and dynamics above 90 km on Mars (Figure 2), we will rely on previous studies and parameterizations for stratospheric and mesospheric formulations. In Yung and DeMore (1999), chapter 7 provides a comprehensive summary of the complex photochemistry, model atmospheres, eddy and molecular diffusion coefficients with altitude, and an explicit specification of 104 reaction rates. The important process of water vapor condensation will be included via parameterization of the photolysis rate vs. altitude profiles in Bertaux and Montmessin (2001). As will be discussed below, our numerical model handles all types of photochemical reactions and processes capable of being represented by an effective reaction rate in a given altitude resolution element (i.e. “within a box” calculations) separately from transport processes (i.e. “between boxes” calculations) in an efficient, yet rigorous manner.

In any scenario for upward coupling in an atmosphere, attention must be given to wave and tidal processes. One of our team members (J. Forbes) has considerable expertise in these areas and, in particular, with new studies for Mars. The Global Scale Wave Model (GSWM) and the Quasi-Nonlinear Model (QNLN), developed for Earth, have now been applied successfully to Mars (Forbes and Hagan 2000; Forbes and Miyahara 2004). This is a complex problem involving multiple coupling processes, including surface topology. The key transport issues relevant to the upward flux of minor species resulting from these processes will be included in our overall model. The BU/FES code to be used (see below) is one that Professor Forbes has used with his students in Colorado, and thus his guidance for its use in the proposed work is a realistic and strong component available to us.

The assumed background atmospheric structure will be consistent with Thermal Electron Spectrometer (TES) and other observations and with lower and upper atmospheric models (eg Haberle et al. 2003; Bougher et al. 1993). In formulating the assumed water content in the atmosphere we will consider observations of sub-surface water reservoirs and their interactions with the atmosphere from Mars Odyssey and Viking Mars Atmospheric Water Detector (MAWD) observations of latitudinal and seasonal variations in column abundance of water vapor. We will compare the cloud structures included in the model to Mars Orbiter Laser Altimeter (MOLA) and imaging system observations of clouds, hazes, and other condensates in the atmosphere. Any assumed dust loading in later stages of the modeling will be consistent with TES observations of latitudinal and seasonal variations in atmospheric dust profiles.

Specific cases of interest that will be studied include:

- Atmospheric water content varies seasonally. How do escape rates respond?
- How do solar cycle variations in incident solar flux affect the escape rates?
- What processes fractionate deuterium from hydrogen and by how much?
- It has been suggested that the Mariner 9 Lyman alpha observations contain day-to-night circulation of atomic hydrogen as well as Jeans-escaping hydrogen (Fox 1993). Are our

results for the thermal escape of hydrogen consistent with the Mariner 9 observations for the case of none, some, or large day-to-night circulation?

- Can our model reproduce accurately the net escape of water from Mars with no change in the planet's oxidation state or do they indicate net reduction or net oxidation of the atmosphere and surface?
- How do escape rates and the nature of the dominant escape processes change if the atmosphere is significantly wetter? This wetter atmosphere could be caused by the introduction of volatiles from volcanic eruptions, breach of confined sub-surface aquifers, or impact-induced hydrothermal systems (Segura et al. 2002).

Current Modeling Capabilities at Boston University:

During the past decade, our observational science programs have been enhanced by an increasing number of modeling efforts, many of these funded by NASA. Starting with a terrestrial model to simulate the effects arising from chemical releases into the atmosphere (Mendillo et al., 1993), our modeling efforts have grown into a series of specialized simulation codes for atmospheric regions on Earth and other planets in the solar system. These may be summarized as follows:

(1) FES Model for the Earth's Atmosphere. This is a fully numerical "Finite Element Simulation" (FES) code that was developed to study large scale releases of water (H_2O), hydrogen (H_2) and carbon dioxide (CO_2) into the atmosphere. The sources were rocket plumes and Space Shuttle exhaust depositions at various altitudes in a broad spectrum of launch scenarios. In addition, NASA sounding rocket experiments conducted a series of "active experiments" to observe and model the effects of specific gases on ionospheric plasma processes. The FES code thus solved for the diffusion of an arbitrary neutral species, in arbitrary amounts, in any spatial and temporal scenario. Since these molecules are highly reactive, the code handles both dynamics and chemistry for neutrals, ions and electrons (and also negative ions when SF_6 , a high electron-affinity gas, was used in the experiments). To cope with a broad range of altitudes, and therefore changing characteristic times and lengths, the spatial grid is completely flexible (i.e. code versions exist in 1-D, 2-D and 3-D), and a master clock keeps each process (with its own time step) in synch. The FES model has been described in detail in Mendillo et al. (1993). A use of it that is highly relevant to Mars was the successful modeling of CO_2 releases into the terrestrial ionosphere that provoked both plasma depletions and bursts of oxygen airglow (6300 Å) observed in two NASA "RED AIR" sounding rocket experiments (Semeter et al. 1996). Thus, for approximately one hour, the affected portion of the terrestrial ionosphere was transformed into a martian ionosphere, and it was modeled successfully.

We propose now to convert the FES code to Mars and to extend its coverage down to the surface. For the processes of interest (i.e., primarily vertical transport), we will use the 1-dimensional version of the FES code as the most efficient way to handle code development. Numerical stability issues are very well understood for FES, and especially so for the 1-dimensional calculations.

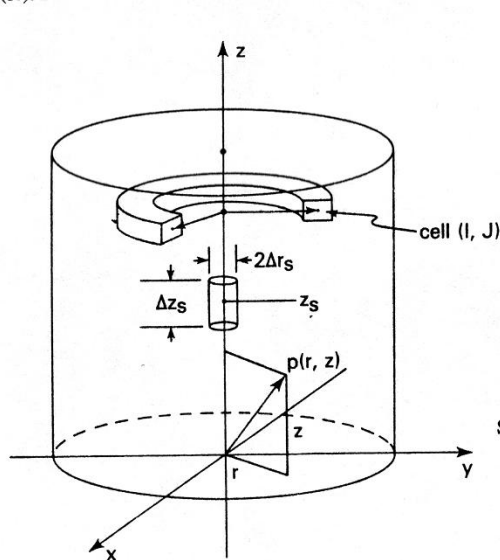


Figure 1: FES cell geometry used to make azimuthally symmetric spatial grid.

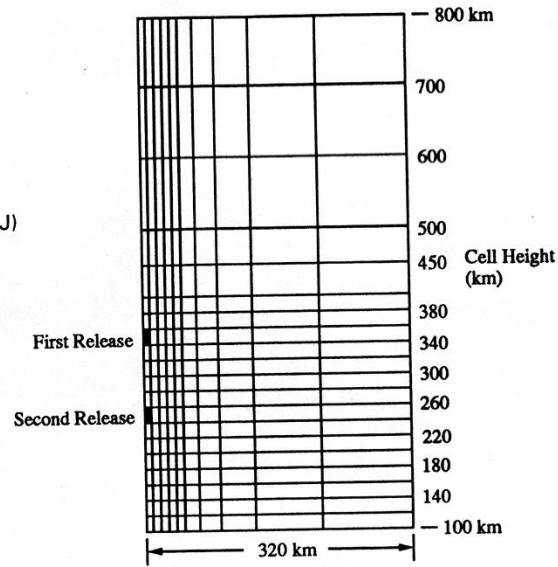


Figure 2: Cross section of spatial grid used to model REDAIR-2. Darkened cells indicate release points.

Figure 3: Schematic of FES model grid with application to RED AIR experiment.

(2) Mars Ionosphere Model (MIM). As part of our Mars Data Analysis Program grant (NASA/MDAP, Mendillo PI) to study thermosphere-ionosphere coupling at Mars, we have successfully simulated day-to-day variability in the martian electron density profiles $N_e(z)$ arising from daily solar irradiance changes (Martinis et al., 2003). The datasets come from the Mars Global Surveyor (MGS) radio science (RS) experiment (Hinson 1999).

The MIM solves the photochemical continuity equation for multiple ions and electrons above 90 km. It includes a state-of-the-art set of solar fluxes, cross sections and reactions rates for 15 atmospheric reactions (neutral and plasma). Recently, MIM has been improved by adding plasma transport thereby allowing for more accurate computation of ionospheric structure above the photochemical peak, i.e., to the topside ionosphere regions of critical importance to studies of escape proposed here (see Figure 4).

(3) Planetary Exosphere Model (PEM). To study the tenuous sodium exospheres of the Moon, Mercury, comet Hale-Bopp, and the complex series of sodium clouds in the Jupiter-Io system, a comprehensive Monte Carlo (M-C) simulation code has been developed. Its versatile capabilities were most recently described for the Moon by Wilson et al. (1999, 2003) and for Io in Wilson et al. (2002). The PEM currently uses the M-C method to handle both the speed distribution and escape rate of atoms at the exobase of the parent body (whether at the surface or at the top of an upper atmosphere). It uses a fourth-order Runge-Kutta integration to calculate the subsequent trajectories, taking into account the gravity of the parent body and the Sun. Solar radiation pressure is included, as well as photo-ionization of the escaping species. The importance of photochemical escape of atomic carbon was demonstrated by Fox and Bakalin

(2001), and the importance of using the Monte Carlo method for its escape (vs. Jean's escape) was stressed by Bakalin and Fox (2002).

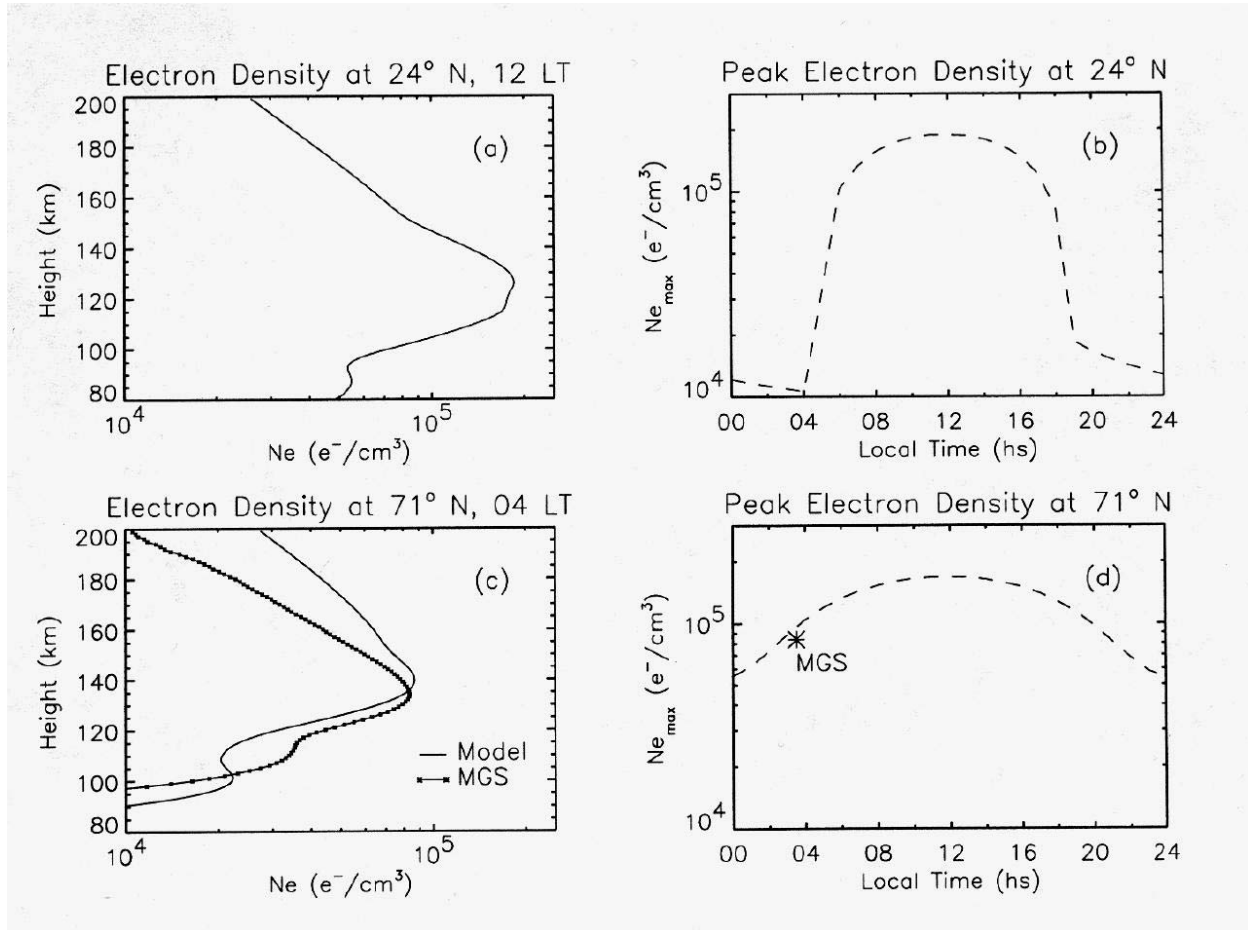


Figure 4: Photochemical model results for the martian ionosphere in March 1999. (a) electron density profile for the sub-solar point; (b) diurnal variation of the peak electron density at the sub-solar point; (c) average electron density profile representative of MGS observations; (d) diurnal variation of average peak electron density at 71 N. An average profile from the MGS observations is also shown in (c) and its peak density in (d). In (c) the model does not match the observed ionospheric profile because diffusion has not been included. When diffusion is included, the fit to the observations is greatly improved.

(4) Modeling the Solar Wind Interaction with the martian upper atmosphere and ionosphere. In addition to the in-house models described above, we have an active collaboration (M. Mendillo, PI) with Dr. Jaqueline Schoendorf (Co-I, Mission Research Corp., Nashua, NH) that is in the process of merging the Mars ionosphere code (MIM) with their MHD simulation code for solar wind flow past a planet. This is, in effect, the final piece in a comprehensive surface-to-solar wind capability for Mars. We will use the results from the solar wind code to address the sputtering rates and pick-up processes needed for the Monte Carlo escape (PEM) code.

Observational Studies of Mars at Boston University:

A recent Hubble Space Telescope (HST) observing program has been carried out at Boston University under PI J. Clarke. Observations at the last two Mars oppositions have been made of D and H Ly alpha emissions at high spectral resolution, and of numerous lines of H, O, and CO at low spectral but high spatial resolution (24 km at Mars). The spectra and distributions of these emissions (see Figure 5) are being published with initial estimates of the escape fluxes which would be consistent with these emission rates and spatial distributions. We therefore have excellent quality observational data with which to constrain the development of detailed models of the escape of H and O from the martian atmosphere. In the analysis of these data, as well, the importance of modeling the entire atmosphere to understand the physical properties has become increasingly clear.

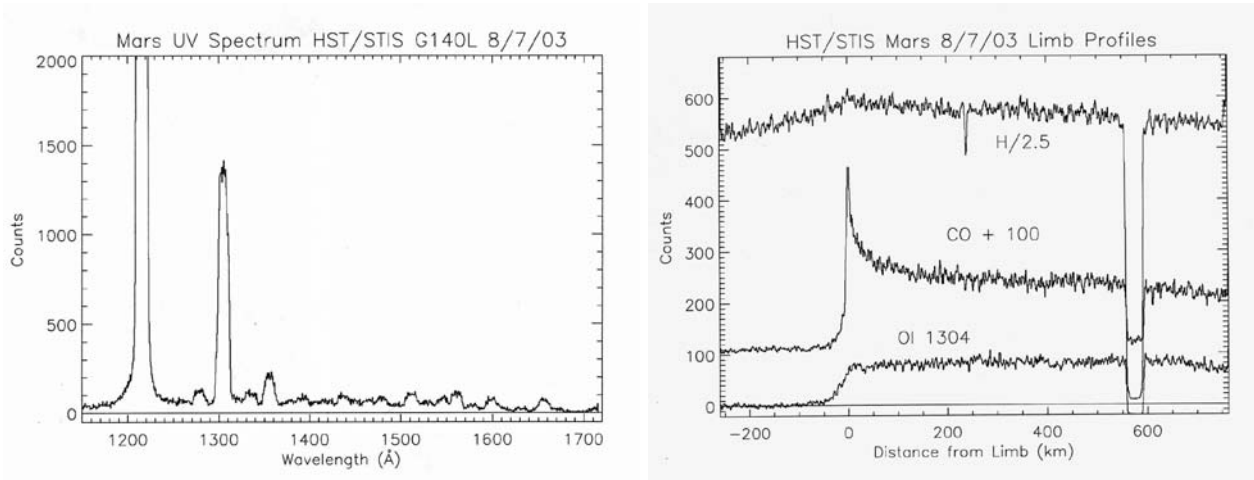


Figure 5: HST/STIS spectrum of martian UV airglow emissions (left) showing principal emissions of H (1216 Å), O (1304, 1356 Å), and CO (1250-1700 Å). Right-hand panel shows the emission intensity across the martian disc for the optically thin CO emissions and optically thick O and H emissions with a spatial resolution of 24 km at Mars, which was achieved during the August 2004 Mars opposition. We also have spectra and spatial profiles of the H and D Ly alpha emissions from HST/STIS obtained during the July 2001 Mars opposition.

Proposed Plan of Work and Schedule:

Building upon our existing capabilities in terrestrial and planetary models for neutral gas diffusion, photochemical processes, atmospheric chemistry, plasma diffusion, and exospheric escape, we propose to merge these methods in a rigorous formulation of a surface-to-exosphere model for Mars. The strategy will be to convert and merge all of the above models into the fully-numerical FES formalism since that allows for the most flexible way to assess (e.g., "turn-on/turn-off") individual processes and mechanisms. The implementation plan is as follows:

Year-1:

- Convert the current analytical Mars Ionospheric Model (MIM) to the FES system. The atmospheric processes in FES and MIM (for Earth and Mars, respectively) are essentially identical, and thus this is the first logical step to make. It will allow for validation since the numerical model results can be checked against the analytical results for the same martian thermosphere-ionosphere.
- Begin the extension of the FES code to include heights below 90 km and input atmospheric constituents down to the surface; conduct trial runs of simple neutral diffusion of test particles.
- Incorporate martian lower atmospheric chemical reactions and condensation parameterization in the FES model.

Year-2:

- Complete the lower atmosphere portion of the model and test dynamical coupling to regions above 90 km.
- Begin coupling of the Planetary Exosphere Model (PEM) to the topside of the surface-to-exobase (0-200 km) model.
- Conduct first tests of surface-to-exosphere escape scenarios.

Year-3:

- Conduct a comprehensive series of simulation scenarios for short and long term effects.
- Assess contributions to escape due to atmospheric sputtering by solar wind particles by parameterizations in the PEM/Monte Carlo calculations.

In terms of computing facilities and support, we have in house an array of Windows machines, Macs, and Sun workstations for use on this project. The Center for Space Physics employs a network administration team for local support and maintenance. We use the resources of the Boston University Office of Information Technology for support in more complicated areas, such as the parallelization of codes for faster run times.

During each year of the project, presentations and progress reports will be made at professional meetings and workshops, and during years 2 and 3 publications of preliminary to final results will be submitted to refereed journals.

Education and Public Outreach:

Few studies enjoy such an inherent fascination with the general public as Mars does. During the opposition period last summer (2003), our Open Night at the Boston University

Observatory (a rooftop teaching facility in downtown Boston) was overwhelmed by 500 visitors! Fortunately, we had anticipated a good turnout, and so three separate functions were conducted simultaneously: a briefing lecture, observing sessions, and NASA videos of Mars exploration with questions and answers. We cycled through these activities for three hours. For the proposed grant period, we plan on building upon this experience with a series of "Mars Nights" throughout the year. Each month, one of the investigators at BU (Clarke, Mendillo, Wilson and Withers) will give a talk, and our graduate student will conduct telescope viewing, (weather and Mars availability cooperating). This will give us a 3-talk responsibility each year, nights certainly well spent on bringing the excitement of Mars research to the public.

In areas of graduate training, we are fortunate that nearly half of the current students in our department are women, and so opportunities for broadening the visibility of woman researchers will be pursued. Boston University is proud that it was the first institution to award the Ph.D. degree to a woman in the US, and our Astronomy Department and the Center for Space Physics has a continuing record of commitment to this important area of advanced training.

Modeling Team Responsibilities:

Under the direction of the PI, a full-time graduate student will conduct the model development as part of dissertation research. Collaborators with expertise in areas central to the model will be available as resources to the PI and graduate student as follows:

- Ionospheric Physics at Mars and FES code development: M. Mendillo
- Specification of lower atmosphere structure and processes: P. Withers and J. Forbes
- Exospheric processes and Monte Carlo techniques: J. Wilson

Program Management:

The PI, Prof. John T. Clarke, will have overall responsibility for oversight of the proposed research, and one month of summer salary each year is requested to support this effort. The PI can supervise the graduate student during the academic year at no cost to this program. The contributions of the Collaborators are described above, and each of these will be at not cost to the proposed grant. Mendillo and Forbes are Professors with independent salary support. Withers and Wilson are Research Associates at Boston University, and have separate research funding for the aspects of this project which require their inputs. They will mainly advise the graduate student, and answer any questions about the implementation of the code. A graduate research assistant will be funded at 100 % for the three years of the proposed research, and this graduate student will work full time on this project as the main subject of their Ph.D dissertation. The Dept. of Astronomy at BU has a large (and academically strong) class of 14 graduate students now finishing their first year of classes, and one of these students will be offered the proposed research topic for their Ph.D thesis. This student will start on the project in Jan. 2005, and will be finished with exams by early May 2005, after which their full efforts will be devoted to this program.

References:

Bakalin, F.M., and J.L. Fox, "Comparison of a Monte Carlo calculation of the escape rate of C from Mars to that obtained using the exobase approximation", abstract, AGU Spring Meeting, EOS, 7 May (2002).

Baker, V., *Nature*, 412, 228-236 (2002).

Barth, C., et al., "Aeronomy of the current martian atmosphere", in *Mars*, pp. 1054-1089, Univ. of Arizona Press (1992).

Belton, M. J. S., et al., "New Frontiers in the Solar System: An Integrated Exploration Strategy", National Research Council (2002); <http://www.nap.edu/catalog/10432.html>.

Bertaux, J.L., and J.T. Clarke, "Deuterium Content of the Venus Atmosphere", *Nature*, 338, 567-570 (1989).

Bertaux, J.L., J.T. Clarke, M.J. Mumma, T. Owen, and E. Quemerais, "A search for deuterium Lyman-alpha emission from the atmosphere of Mars", in *Proc. of the ST-ECF/STScI Workshop: Science with the Hubble Space Telescope*, ed. P. Benvenuti and E. Schreier, pp. 459-465 (1992).

Bertaux, J.L., and F. Montmessin, "Isotopic fractionation through water vapor condensation: the Deuteropause, a cold trap for deuterium in the atmosphere of Mars", *J. Geophys. Res.*, 106, E12, 32,879-32,884 (2001).

Bougher, S. W., C. G. Felsen, E. C. Ridley, and R. W. Zurek "Mars mesosphere and thermosphere coupling - Semidiurnal tides", *J. Geophys. Res.*, 98, 3281-3295 (1993)

Chamberlain, J. W, and D. M. Hunten , "Theory of Planetary Atmospheres", Academic Press (1987).

Donahue, T. M., D. H. Grinspoon, R. E. Hartle, and R. R. Hodges, "Ion/Neutral Escape of Hydrogen and Deuterium: Evolution of Water" 385-414, in *Venus*, ed.s S.W. Bougher, D. M. Hunten, and R. J. Phillips (1997).

Forbes, J.M., and M. E. Hagan, "Diurnal Kelvin wave in the thermosphere of Mars: Towards an understanding of 'stationary' density structures observed by the MGS accelerometer," *Geophys. Res. Lett.*, 27, 3563-3566, 2000.

Forbes, J. M., and S. Miyahara, "Tide-mean flow interactions in the upper atmospheres of Earth and Mars", EGU Annual Meeting, Nice, France, April, 2004.

Forbes, J. M., "Wave coupling in terrestrial planetary atmospheres", in *Atmospheres in the Solar System: Comparative Aeronomy* (M. Mendillo, A. Nagy, J.H. Waite, eds), *AGU monograph #130*, 171-190, 2002.

Fox, J.L., "On the escape of oxygen and hydrogen from Mars", *Geophys. Res. Lett.* 20, 1747-1750 (1993).

Fox, J.L., "Upper limits to the outflow of ions at Mars: Implications for atmospheric evolution", *Geophys. Res. Lett.* 24, 2901 (1997).

Fox, J.L., and F.M. Bakalian "Photochemical escape of atomic carbon from Mars", *J. Geophys. Res.* 106, 28785-28796 (2001).

Fox, J. L., "Effect of H₂ on the Martian ionosphere: Implications for atmospheric evolution", *J. Geophys. Res.*, 108, A6, 1223, doi:10.1029/2001JA000203 (2003).

Haberle, R. M., J. R. Murphy, and J. Schaeffer "Orbital change experiments with a Mars general circulation model", *Icarus*, 161, 66-89 (2003).

Hinson, D.P., R.A. Simpson, J.D. Twicken, and G. L. Tyler, "Initial results from radio occultation measurements with Mars Global Surveyor", *J. Geophys. Res.*, 104, 26997-27012 (1999).

Hunten, D.M., "Atmospheric evolution of the terrestrial planets", *Science* 259, 915-920 (1993).

Jakosky, B.M., and R.J. Phillips, "Mars' volatile and climate history", *Nature*, 412, 237-244 (2001).

Johnson, R.E., and J.G. Luhmann, "Sputter contribution to the atmospheric corona on Mars", *J. Geophys. Res.*, 103, E2, 3649-3653 (1998).

Krasnopolsky, V.A., M.J. Mumma, and G.R. Gladstone, "Detection of atomic deuterium in the upper atmosphere of Mars", *Science*, 280, 1576 (1998).

Krasnopolsky, V.A., "Mars' upper atmosphere and ionosphere at low, medium, and high solar activities: Implications for evolution of water", *J. Geophys. Res. (Planets)* 11-1, (2002).

Lewis, J.S., "Physics and Chemistry of the Solar System", Academic Press (1997).

Martinis, C.R., J.K. Wilson, and M. Mendillo, "Modeling day-to-day ionospheric variability at Mars", *J. Geophys. Res.*, 108, A10, 1383, doi:10.1029/2003JA009973 (2003).

McElroy, M. B., "Mars: an evolving atmosphere", *Science*, 175, 443 (1972).

Mendillo, M., J. Semeter, and J. Noto, "Finite element simulation (FES): A computer modeling technique for studies of chemical modification of the ionosphere", *Adv. Space Res.*, 13(10), 55-64 (1993).

Nair, H., M. Allen, A. D. Anbar, Y. L. Yung, and R. T. Clancy "A Photochemical Model of the Martian Atmosphere", *Icarus* 111, 124-150 (1994).

Nier, A. O., and M.B. McElroy, "Composition and structure of Mars' upper atmosphere - Results from the neutral mass spectrometers on Viking 1 and 2", *J. Geophys. Res.*, 82, 4341-4349 (1977).

Segura T. L., O. B. Toon, A. Colaprete, and K. Zahnle, "Environmental Effects of Large Impacts on Mars", *Science*, 298, 1977-1980 (2002).

Semeter, J., M. Mendillo, J. Baumgardner, J. Holt, D. Hunton and V. Eccles, "A study of oxygen 6300 A airglow production through chemical modification of the nighttime ionosphere", *J. Geophys. Res.*, 101, A9, 19683-19699 (1996).

Wilson, J.K., J. Baumgardner, and M. Mendillo, "The Outer limits of the lunar sodium exosphere", *Geophys. Res. Lett.*, 30, 12, 1649, doi:10.1029/2003GL017443 (2003).

Wilson, J.K., M. Mendillo, J. Baumgardner, N. Schneider, J.T. Trauger, and B. Flynn, "The dual sources of Io's sodium clouds", *Icarus*, 157, 476-489 (2002).

Wilson, J.K., S.M. Smith, J. Baumgardner, and M. Mendillo, "Modeling an enhancement of the lunar sodium atmosphere and tail during the Leonid meteor shower of 1998", *Geophys. Res. Lett.*, 26, 1645-1648 (1999).

Yung, Y.L., and D. Kass, "Deuteronomy?: A puzzle of deuterium and oxygen on Mars", *Science*, 280, 1545-1546 (1998).

Yung, Y.L., and W.B. DeMore, "Photochemistry of Planetary Atmospheres", Oxford Univ. Press (1999).